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Electrical Resistivity Studies of Order-Disorder Phenomena in V2H and V2D

Gust Bambakidis
Wright State University - Main Campus, gust.bambakidis@wright.edu

M. W. Pershing

R. C. Bowman

(TSH) in these bcc alloys. The TSH's, which are marked by the onset of hydride precipitation from the saturated solid solution, were determined resistometrically from discontinuities in dρ/dT. Increases in the apparent TSH in Nb-Ti alloys are believed to be due to the presence of energetically favorable interstitial sites, or "traps", in the vicinity of the substitutional Ti solute atoms. The magnitude of the TSH enhancements suggests that Ti is a more effective trapping center than Ta, but less effective than V. Proposed explanations for this behavior based upon electronic and atom-size considerations will be discussed.

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KJ 6 Electrical Resistivity Studies of Order-Disorder Phenomena in V_2H and V_2D. G. BAMBAKIDIS and M.W.PERSHING* Wright State University, and R. C. BOWMAN, JR., Mound Facility**.--There is a marked isotope effect in the V-H (D) phase diagrams. The disordering of the H(D) on the octahedral sublattice in the β phase is different for V-H and V-D. From the non-linearity in the ρ versus T curves for $V_2H(D)$ we have obtained the temperature variation of the LRO parameter for H and D. For V_2H the results indicate a second-order transition within the β phase before the onset of the α phase. The LRO parameter agrees closely with that inferred from powder neutron diffraction measurements[1]. For V_2D a first-order β→α transition is indicated. Our LRO parameter in this case differs significantly from the neutron diffraction results[2] but agrees well with that inferred from X-ray diffraction[3].

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[2]H. Asano et al, Paris Cong. H_2 in Mets. (1977).
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KJ 7 X-dependent Optical Studies of LaH_x. D. J. PETERMAN, D. T. PETERSON, Ames Laboratory-USDOE* and J. H. WEAVER, Synchrotron Radiation Center, University of Wisconsin-Madison.--Optical absorptivity experiments in the photon energy range of 0.2-4.5 eV for various concentrations of hydrogen in CaF_2-structured LaH_x have been performed. The measured quantities were used to determine the frequency-dependent dielectric functions. The results have been interpreted in light of previous experimental and theoretical studies of the electronic structure of ScH_2 and YH_2.[1,2] Based on the results of that earlier work, one would expect hydrogen to occupy a substantial number of octahedral sites in LaH_2 - perhaps giving rise to 'new' interband transitions. Such transitions have been observed and their concentration dependence allows us to classify the observed interband transitions as to whether or not they arise from octahedral site occupation.

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KJ 8 Sample Shape-Dependent Phase Transition of Hydrogen in Niobium, H. ZABEL, University of Houston*, H. PEISL, University of Munich.**--The α-α' phase transition of hydrogen in Niobium closely resembles a gas-liquid transition of a real gas. The hydrogen atoms interact mainly via the long range elastic distortion field of the host metal atoms. The theory of elastic interaction and phase transition in coherent metal-hydrogen systems[1] predicts strongly depressed critical fluctuations at the critical point (c_c = 0.31 H/Nb, T_c = 171°C). Only a few modes become unstable below T_c on isochoral cooling of Nb samples, after in situ loading with hydrogen above T_c. It will be shown by means of X-ray scattering that those modes vary macroscopically over the whole sample size. The density modes depend sensitively on the sample geometry due to the fulfillment of the elastic boundary condition. Coherent hydrogen fluctuations are observed down to 40 degrees below T_c.

*Supported by U.S. DOE Contract EY-76-S-05-5111
**Supported by Bundesministerium fur Forschung and Technologie

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KJ 9 Phase Equilibria and Hydrogen Trapping in Dilute Alloys of Vanadium in Niobium.* M. A. PICK and D. O. WELCH, Brookhaven Nat'l. Lab.--The effect of dilute vanadium additions to niobium on hydrogen absorption was studied by measuring the temperature dependent equilibrium hydrogen partial pressure for pure Nb, Nb+6at.%V, and Nb+9at.%V. A theoretical model of the effect of hydrogen trapping on phase equilibria in the α-α' region of such systems was constructed. The results indicate that the H-V binding energy is less than previously thought.[1] A value of .07 eV is obtained from the depression of the α-α' critical temperature, but the shape of the pressure isotherms suggests that this is an upper limit. The measured heat of solution decreases from -37.0 to -38.6 to -38.8 kJg-atom^{-1} going from pure Nb to Nb+6at.%V to Nb+9at.%V.

*Research supported by the Div. of Basic Energy Sciences of DOE.

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KJ 10 Heat Capacity and Disorder in ScD_x.* MARVIN MOSS, Sandia Labs.†— Excess heat capacity in ScD_x ($x = 0\text{-}1.83$) in the range 298-1000 K is greatest for $x \approx 1$. This can be explained by a disorder model which has been applied to cation-disordered phases in which a larger number of sites than mobile species leads to a configurational contribution to the entropy.[1] It is assumed that high-energy interstitial sites are created by the introduction of deuterium,[2] the occupation of the sites being temperature dependent. A two-level model for site energies leads to maxima in the entropy and heat capacity for mid-range values of x.

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† A U.S. DOE facility.

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2 A. L. G. Rees, Trans. Faraday Soc. 50, 335 (1954).

KJ 11 Evidence for Ordered Octahedral Protons Around Dilute Er in YH_x.* E. L. VENTURINI, Sandia Labs.**--We present evidence for ordered arrangements of octahedral protons around dilute Er ions in YH_x using electron spin resonance (ESR) of the Er in powdered hydride samples. When the hydrogen to metal ratio x is less than 2, we observe an isotropic ESR signal plus two distinct uniaxial resonances. The isotropic signal arises from an Er ion with eight nearest-neighbor tetrahedral protons (cubic site symmetry), and the uniaxial resonances correspond to Er ions with either one or two additional next-nearest-neighbor octahedral protons. A sample of $YH_{2.4}$:Er shows a new ESR signal from a site with biaxial symmetry (three unique axes) plus the isotropic signal from Er in a cubic site, but not the uniaxial site resonances just discussed. We have tentatively identified the biaxial Er site as the mer-XA_3 structure recently reported for stoichiometric $PrD_{2.5}$. In this structure all eight tetrahedral proton sites are filled, and there are three ordered octahedral protons.

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KJ 12 Proton Distribution in Vicinity of a Rare Earth Impurity in a Hydride.* P.M. RICHARDS, Sandia Labs.** Recent ESR and earlier Mössbauer studies of dilute Er